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Dealing with the Quaternion Antipodal Problem for Advecting Fields

by Richard Becker

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by Richard Becker
Weapons and Materials Research Directorate, ARL

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14. ABSTRACT
Quaternion representations of rotations are proposed for advecting rotations in large strain simulations. One algorithm enforces continuity to resolve the ambiguity created by equivalent antipodal representations and the other proposes using products of quaternions to ameliorate these issues. The results of both are unique and continuous, but the former does not capture the correct periodicity and the latter requires special treatment for 180° rotations.

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1. Introduction

In multi-physics codes simulating large material flows, representations of the underlying material structure must transport through the computational grid. Material enters and leaves computations cells. Quantities like energy, density, and material state are determined by a weighted average of the state entering a cell and what remains after material exits. Errors are introduced by advecting structure variables through the grid, and algorithms minimizing these errors improve the quality of the solution. For solid mechanics, one of the more challenging quantities to advect is the deformation gradient tensor because nonlinear combinations of the 9 components correspond to physical quantities. For example, the determinant of the deformation gradient describes the volume change. There is little chance that a linear combination of the 9 individual components of 2 deformation gradients will yield the same determinant as taking the linear combination of the determinants.

One strategy to reduce advection error is to decompose the deformation gradient, $\mathbf{F}$, into smaller, physically meaningful pieces and to advect those. The multi-step decomposition being investigated at the US Army Research Laboratory (ARL) begins with an $\mathbf{F} = \mathbf{RU}$ decomposition of the deformation gradient, where $\mathbf{R}$ is an orthogonal rotation matrix and $\mathbf{U}$ is the symmetric right stretch tensor. The focus of this technical brief is on advection of the rotation.

Rotation of an object or a microstructure can be represented in many forms, such as Euler angles,[1] angle-axis pairs, Rodrigues vectors,[2] quaternions and rotation matrices.[3,4] While 3 parameters are sufficient to define a rotation, as in Euler angles, more parameters are often used for convenience or other reasons. Consider, for example, an angle-axis pair, which is defined in terms of a rotation ω about the unimodular axis $\mathbf{c}$. While there appear to be 4 parameters, the axis is a unit vector, so there is an additional constraint, leaving only 3 independent parameters. Likewise, a quaternion representation has 4 parameters and a constraint equation. A rotation matrix has 9 parameters, with 6 constraints from the orthogonality requirement. Advecting large numbers of redundant parameters is not ideal since they must be adjusted consistently after advection to satisfy the constraint equations.

From the perspective of having no redundant parameters, Euler angles and Rodrigues vectors both appear suitable. However, Euler angles are not periodic with continued rotation. A body is in an identical orientation after a 360° rotation about

an axis, but the Euler angles do not naturally return to the same values. A step change in angles is necessary to keep the angles within a fundamental range. The lack of periodicity is not an issue for many applications, but advection requires a continuous parameterization, so Euler angles are not suitable for current considerations. Rodrigues vectors, on the other hand, use periodic functions. However, the components are unbounded as the cosine function in the denominator passes through zero. A singularity cannot be accommodated so Rodrigues vectors are also not suitable in the current context.

Angle-axis pairs and quaternions both have one redundant parameter. Similar to Euler angles, the angle-axis pairs suffer from inability to represent periodicity in rotations. The angle continuously increases with rotation. Quaternions are built on periodic functions and are bounded. In addition, errors introduced by noise in quaternions are less severe than for other methods,[5] such as Euler angles, so there is additional incentive for their use. Methods based on quaternions will be explored in further detail in this report.

2. Quaternion Representation of a Rotation Matrix

The rotation of a body can be represented in terms of a rotation, ω, about a unimodular axis, $\mathbf{c}$. Quaternions are related to angle-axis pairs, but they employ cyclic functions that are able to capture periodicity. In terms of the rotation angle, ω, and axis, $\mathbf{c}$, the 4 components of the quaternion are defined in a rectangular Cartesian coordinate system as

$$\begin{aligned} \lambda &= c_1 \sin(\omega/2) \\ \mu &= c_2 \sin(\omega/2) \\ \nu &= c_3 \sin(\omega/2) \\ \rho &= \cos(\omega/2) \end{aligned} \quad , \tag{1}$$

subject to the constraint

$$\lambda^2 + \mu^2 + \nu^2 + \rho^2 = 1 \quad . \tag{2}$$

Quaternions can be used to construct the rotation matrix, $\mathbf{R}$, uniquely by

$$R_{ij} = \begin{bmatrix} \lambda^2 - \mu^2 - \nu^2 + \rho^2 & 2(\lambda\mu - \nu\rho) & 2(\nu\lambda + \mu\rho) \\ 2(\lambda\mu + \nu\rho) & \mu^2 - \nu^2 - \lambda^2 + \rho^2 & 2(\mu\nu - \lambda\rho) \\ 2(\nu\lambda - \mu\rho) & 2(\mu\nu + \lambda\rho) & \nu^2 - \lambda^2 - \mu^2 + \rho^2 \end{bmatrix} . \quad (3)$$

When determining quaternions from a rotation matrix, there is a nonuniqueness as 2 sets of quaternions can be determined for any general rotation matrix. Inspection of Eq. 3 reveals that a sign indeterminacy stems from the quaternions only appearing as products. Changing the sign on all of the quaterions gives the same rotation. Redundancy is also expected because of the half angle in Eq. 1; it takes 2 full rotations to run the range of the periodic functions. A common means of dealing with this problem is to ensure that one of the quaterion components is always positive. While this guarantees a unique solution acceptable for many applications, it forces a discontinuous sign change in other components. The discontinuity could create issues if quaternions are used to advect a rotation.

Figure 1 shows examples of quaternion components for 400° rotations of 2 different initial rotation matrices. The cosine component, ρ, was forced to be positive. As ρ hits zero, where there would have been a sign change, other quaternion components flip sign creating large discontinuities.

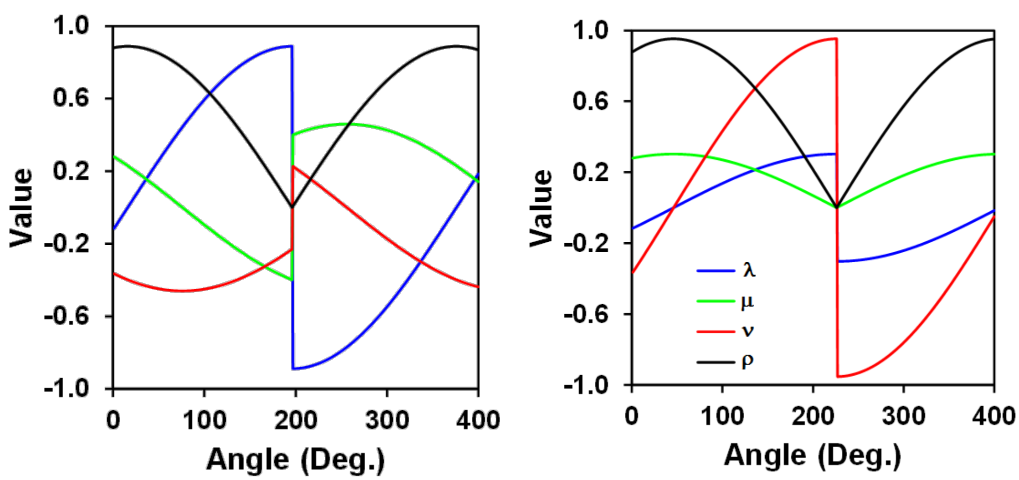

Fig. 1 Evolution of quaternion components for 2 different initial rotation matrices

Had another of the quaternion components been chosen to be always positive, the discontinuity would have occurred in another place.

3. Continuity from Evolution

Continuity conditions can be applied to evolve the quaternions if the rotations are associated with the deformation gradient. The deformation gradient begins as the identity and evolves continuously over time. Generally, the deformation gradient at the beginning of the time step will be available when the deformation gradient at the end of the step is calculated. This allows selection of the sign on the quaternion to keep the values continuous. Within a finite element code, as long as the deformation gradients in neighboring elements continue to evolve smoothly, discontinuities should never exist between adjacent elements. Barton[6] has used the sign of the inner product of the beginning-of-step and end-of-step quaternions to trigger a sign flip.

$$\rho_0\rho + \lambda_0\lambda + \mu_0\mu + \nu_0\nu < 0 \quad . \tag{4}$$

If the inner product is negative, the sign of all of the quaternion components is changed. The rotations shown in Fig. 1 are recalculated using sign continuity, and the results are shown in Fig. 2. The quaternions are now continuous throughout the range.

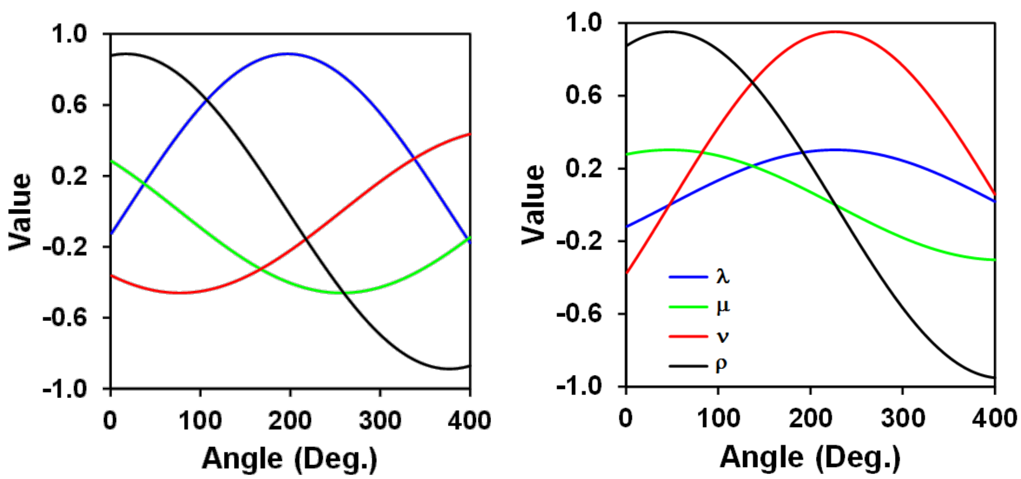

Fig. 2 Evolution of quaternion components for 2 different initial rotation matrices using continuity from previous value

This continuity criterion is particularly well suited for the deformation gradient, where, initially, $\rho = 1$ and $\lambda = \mu = \nu = 0$. The sum in Eq. 4 is dominated by ρ in the vicinity of the initial orientation, and no sign change will be indicated. The remaining values transition smoothly from positive to negative. Other quaternion components dominate Eq. 4 at large rotations to maintain continuous values.

While the method ensures continuity, not all symmetries are captured. Consider 2 material points with common material directors. After rotating each 180° in opposite directions, they will again have a common orientation. However, the sine portion of the quaternions in Eq. 1 will have opposite algebraic signs and will not show the proper orientation relationship. The half angles create a parameter space that is twice the size needed, and the functions do not cycle back on themselves at the correct rate.

The criterion also does not resolve ambiguities in other initial rotations. Say the initial rotation is 180° about the z-axis. The first 2 diagonal elements of the rotation matrix are -1 and the off-diagonals are zero. Perturbations on one side of this have the product $\rho\nu$ being positive and the product is negative for perturbations on the other side. The signs of ρ and ν individually are not determined without introduction of additional rules. If ρ is assumed positive, as in the case of the initial rotation being the identity, the ν will be discontinuous between positive and negative rotating points. Alternative rules would have to be applied in such situations.

It is not anticipated that the deficiencies noted above will be an issue for the deformation gradient, but such situations may arise for the lattice orientations in crystal plasticity simulations. Alternative methods may be useful for the more general case.

4. Proposal for a Unique Representation

The solution proposed here is to retain the quaternion products from the rotation matrix so that unique determination of the algebraic sign is not necessary. Hence, the products $\lambda\rho$, $\mu\rho$, $\nu\rho$, and ρ^2 are advected. There is an obvious issue when $\rho = 0$ and all of the component products to be advected are zero. The proposed solution includes a lower limit on ρ such that $\rho^2 \geq \epsilon^2$ for some small ϵ. With this condition, the quantities advected are $\lambda\tilde{\rho}$, $\mu\tilde{\rho}$, $\nu\tilde{\rho}$, and $\rho\tilde{\rho}$, where

$$\tilde{\rho} = \begin{cases} \rho & \text{if} \quad \rho^2 \geq \epsilon^2 \\ \epsilon & \text{otherwise} \end{cases} \quad . \tag{5}$$

Given a rotation matrix, the procedure is to first determine

$$\rho^2 = \frac{1}{4}\left(R_{11} + R_{22} + R_{33} + 1\right) \quad , \tag{6}$$

and compare the value with ϵ^2. If $\rho^2 \geq \epsilon^2$, then

$$\begin{aligned}
\lambda\tilde{\rho} &= \frac{1}{4}\left(R_{32} - R_{23}\right) \\
\mu\tilde{\rho} &= \frac{1}{4}\left(R_{13} - R_{31}\right) \\
\nu\tilde{\rho} &= \frac{1}{4}\left(R_{21} - R_{12}\right) \\
\rho\tilde{\rho} &= \rho^2
\end{aligned} \quad . \tag{7}$$

If $\rho^2 < \epsilon^2$ the rotation matrix diagonal is used to compute components as:

$$\begin{aligned}
\lambda\tilde{\rho} &= \frac{1}{2}\epsilon \operatorname{sign}\left(R_{32} - R_{23}\right)\sqrt{+R_{11} - R_{22} - R_{33} + 1} \\
\mu\tilde{\rho} &= \frac{1}{2}\epsilon \operatorname{sign}\left(R_{13} - R_{31}\right)\sqrt{-R_{11} + R_{22} - R_{33} + 1} \\
\nu\tilde{\rho} &= \frac{1}{2}\epsilon \operatorname{sign}\left(R_{21} - R_{12}\right)\sqrt{-R_{11} - R_{22} + R_{33} + 1} \\
\rho\tilde{\rho} &= \epsilon\sqrt{\rho^2}
\end{aligned} \quad . \tag{8}$$

This latter case only applies when rotation angles are near 180°, where $\lambda^2 + \mu^2 + \nu^2 \simeq 1$ and the magnitude of the advected quantities is set by the parameter ϵ.

Following advection, limits should be imposed on the advected values and the constraint equation must be applied to ensure valid values and a pure rotation. Since each of the quaternion factors is bounded between -1.0 and 1.0, the advected quaternion products ($\lambda\tilde{\rho}$, $\mu\tilde{\rho}$, $\nu\tilde{\rho}$, and $\rho\tilde{\rho}$) are also bounded between -1.0 and 1.0. Application of the constraint from Eq. 2 determines the scaling factor, $\tilde{\rho}^{*2}$, through

$$\tilde{\rho}^{*2} = (\lambda\tilde{\rho})^2 + (\mu\tilde{\rho})^2 + (\nu\tilde{\rho})^2 + (\rho\tilde{\rho})^2 \quad . \tag{9}$$

Dividing through Eq. 9 by $\tilde{\rho}^{*2}$, it can be seen that the ratio $\tilde{\rho}^2/\tilde{\rho}^{*2}$ multiplies each of the quaternion values to satisfy the constraint. If there are no advection errors the ratio is 1.0. The quaternion products needed to reconstruct the rotation matrix can then be obtained without loss of sign information from the advected quantities and the scaling factor, $\tilde{\rho}^{*2}$, using

$$\lambda^2 = \frac{(\lambda\tilde{\rho})^2}{\tilde{\rho}^{*2}}\,, \qquad \lambda\mu = \frac{\lambda\tilde{\rho}\,\mu\tilde{\rho}}{\tilde{\rho}^{*2}}\,, \qquad \text{and} \qquad \rho^2 = \frac{(\rho\tilde{\rho})^2}{\tilde{\rho}^{*2}} \quad . \tag{10}$$

Similar expressions are applied to determine the remaining terms. These quantities can be used directly in Eq. 3 to calculate the rotation matrix. The value of $\tilde{\rho}^{*2}$ will be nonzero unless advection error results in all 4 advected quaternion products being zero. The limiting value, ϵ, was introduced to prevent a zero solution, but it should be guarded against in the algorithm nonetheless. This can be ensured by enforcing $\tilde{\rho}^{*2} \geq \epsilon^2$ when evaluating Eq. 9 by scaling each of the terms on the right hand side. It is critical that the values used in Eq. 10 satisfy Eq. 9.

Using the representation in Eq. 7 and Eq. 8, the 4 advected components are plotted in Fig. 3 for the same rotations as in Fig. 1. It can be seen that the functions are smooth and continuous. One of the points in each figure has $\rho\tilde{\rho} = 0$ identically, and the other quantities are nonzero because of the ϵ offset.

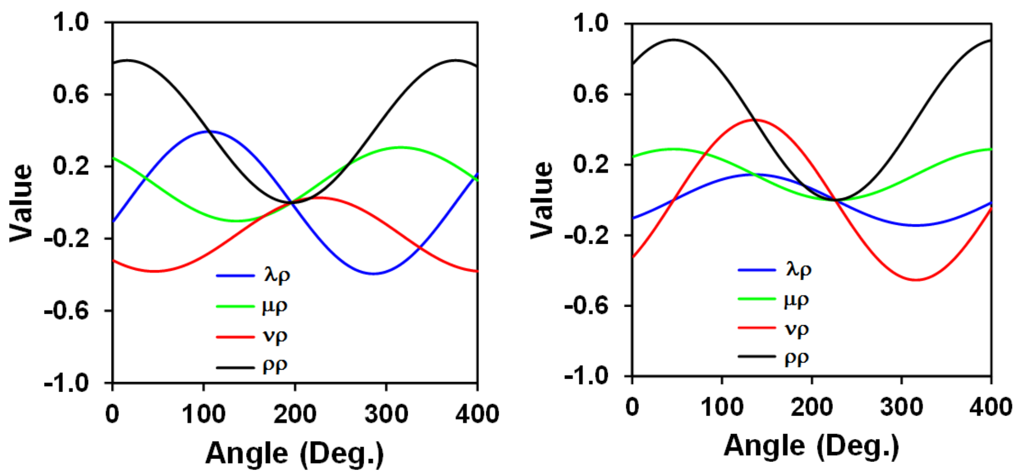

Fig. 3 Evolution of quaternion products for 2 different initial rotation matrices

It is interesting that the quaternion products proposed create a representation in terms of the full rotation angle from an angle-axis pair rather than the half angle shown in Eq. 1. The products are:

$$
\begin{aligned}
\lambda\rho &= c_1 \sin(\omega/2)\cos(\omega/2) = \frac{1}{2}\,c_1 \sin(\omega) \\
\mu\rho &= c_2 \sin(\omega/2)\cos(\omega/2) = \frac{1}{2}\,c_2 \sin(\omega) \\
\nu\rho &= c_3 \sin(\omega/2)\cos(\omega/2) = \frac{1}{2}\,c_3 \sin(\omega) \\
\rho\rho &= \cos^2(\omega/2) = \frac{1}{2}\left[1 + \cos(\omega)\right]
\end{aligned}
\quad . \qquad (11)
$$

Here the angular range for periodicity corresponds to the physical rotation. The angular range for periodicity for quaternions, on the other hand, is twice that of the physical rotation. Keeping the correct angular range eliminates the antipodal problem. However, the representation in Eq. 11 does not have a simple form for the constraint equation, as Eq. 9 involves both ρ^2 and ρ^4.

The troublesome special cases described with the continuity approach in Section 3 do not create the same issues with the proposed representation. Since the full rotation angle is used in Eq. 11 rather than the half angle, 2 material points rotated 180° in opposite directions will have the same representation. In addition, initial orientations of 180° are zero, so there will not be discontinuous behavior at these points.

The potential issue with the proposed representation is the method to avoid the singularity when ρ is zero. This will require further exploration and use to uncover any difficulties.

5. Summary and Conclusions

Two methods are explored for dealing with the antipodal ambiguity in representing rotations by quaternions. Enforcing continuity between beginning and end step values should work well for rotations associated with the deformation gradient. An alternative method based on the sine of the full rotation angle is proposed for situations where continuity cannot be enforced or for more arbitrary initial orientations.

6. References

1. Euler L. Formulae generales pro translatione quacunque corporum rigidorum. Novi Comm Acad Sci Imp Petrop. 1775;20:189.

2. Rodrigues O. Des lois géométriques qui régissent les déplacements d'un système solide dans l'espace, et de la variation des coordonnées provenant de ses désplacements considérés indépendamment de causes qui peuvent les produire. J. de Mathématiques Pures et Appliquées. 1840;5:380.

3. Altmann SL. Rotations, quaternions and double groups. 1st ed. Oxford, U.K.: Oxford University Press; 1986.

4. Becker R, Panchanadeeswaran S. Crystal rotations represented as rodrigues vectors. Textures and Microstructures. 1989;10:167-194.

5. Krieger-Lassen N, Juul-Jensen D. On the statistical analysis of orientation data. Acta Cryst. A. 1994;50:741-748.

6. Barton N. Lawrence Livermore National Laboratory, Livermore, CA., Private email communication. 2017 July 19.

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